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DRACO and Nonequilibrium Statistical Mechanics of Aging

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Outline

- Types of problems which DRACO was designed to address
- Tools from nonequilibrium statistical mechanics:
- Rare events (Extreme value statistics)
- Transients (Diverging time scales)
- Thresholds (Absorbing phase transitions)

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Slide 2

- $A + X \xrightarrow{k_1} 2X$

$X + Y \xrightarrow{k_2} 2Y$

$Y \xrightarrow{k_3} B$

1

2

3

+

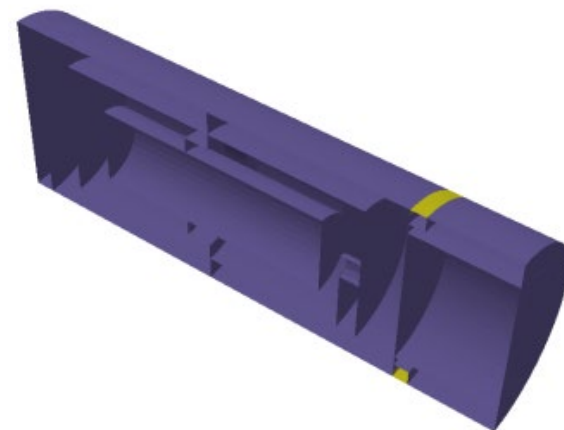
$$\frac{da(t)}{dt} = -k_1 a(t)x(t)$$

$$\frac{db(t)}{dt} = -k_2 b(t)y(t)$$

$$\frac{dx(t)}{dt} = -k_1 a(t)x(t) + k_2 b(t)y(t)$$

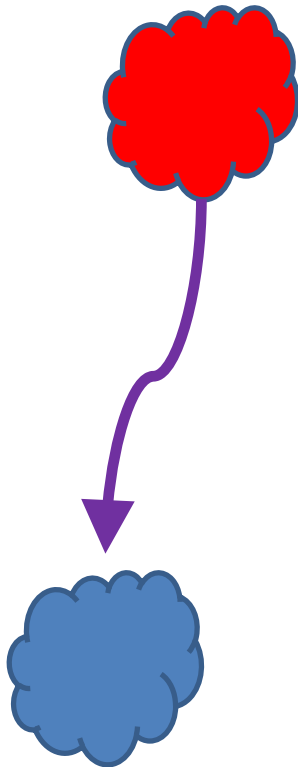
$$\frac{dy(t)}{dt} = k_1 a(t)x(t) - k_2 b(t)y(t)$$

+



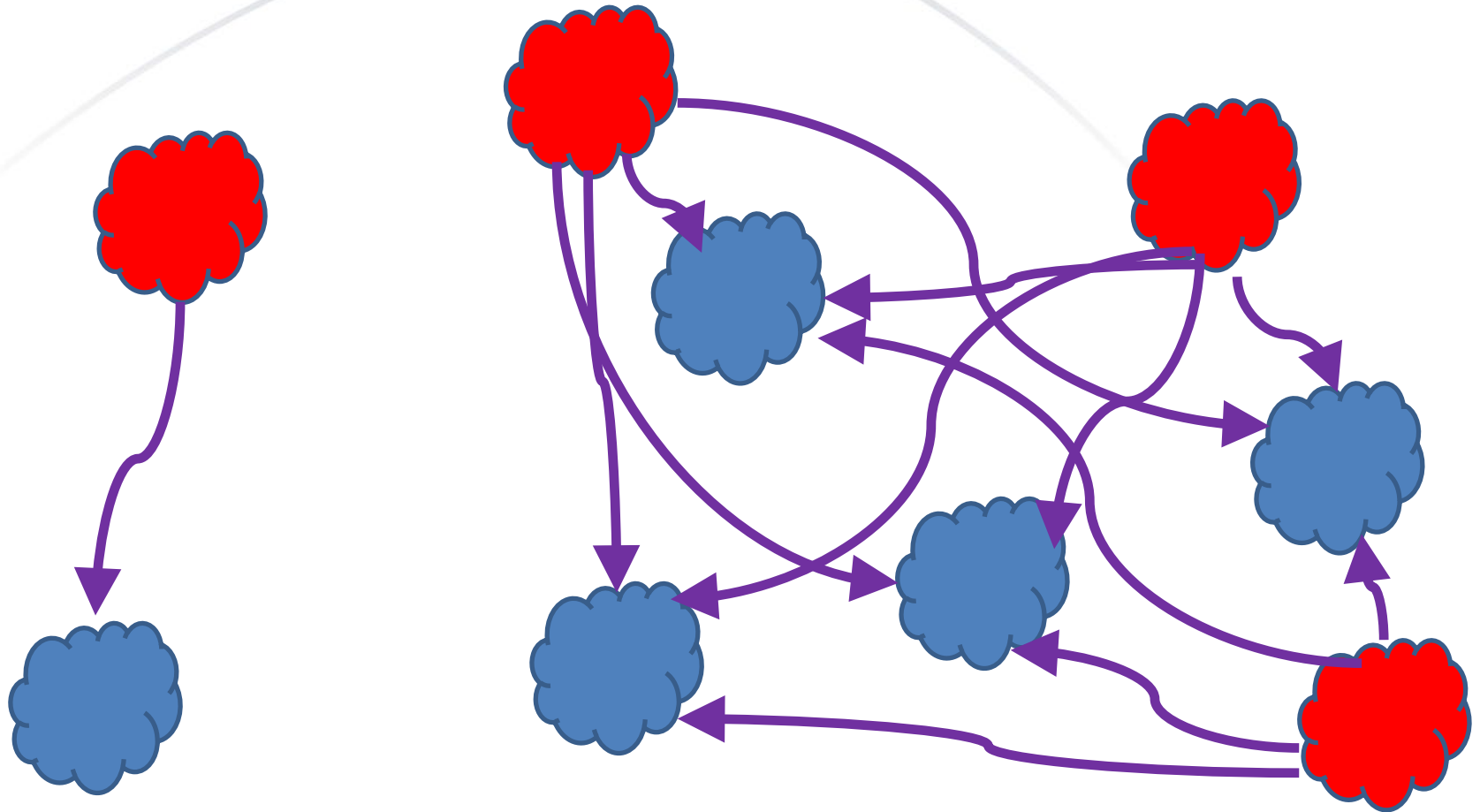
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Gas flow



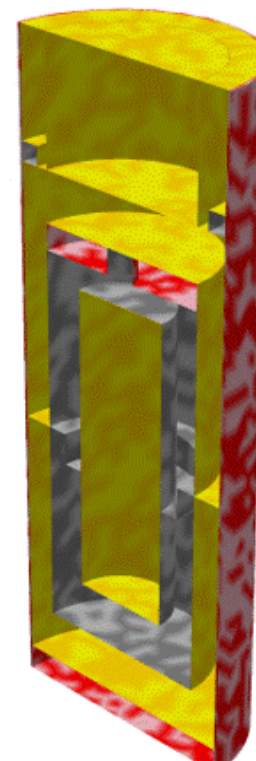
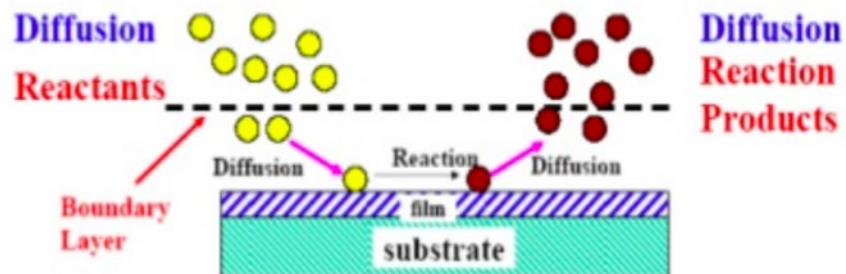
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Gas flow



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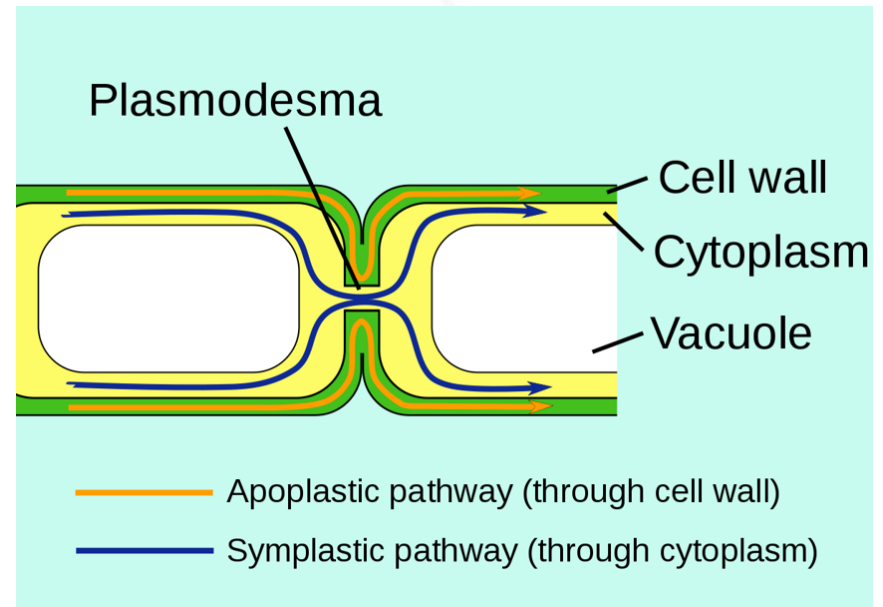
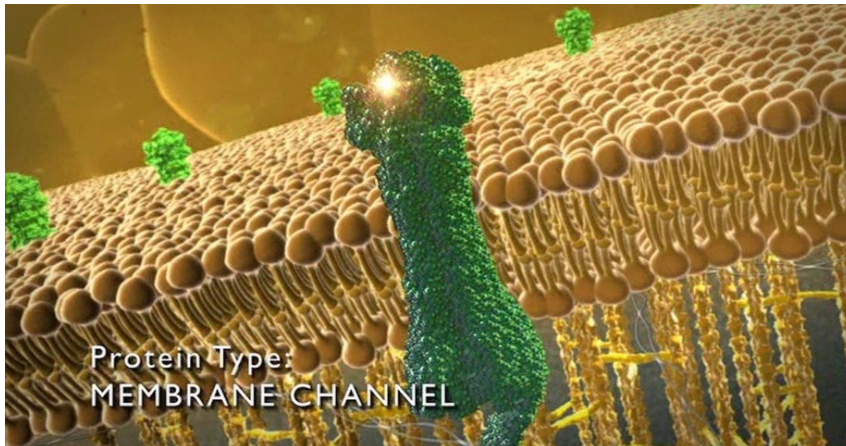
Multiscale geometry in DRACO



Constrained diffusion. Reactions in bulk and at surface.

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Constrained transport is common in biology



Diffusion has different properties in 3D, 2D, and 1D

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DRACO is the best tool when:

- Diffusion constrained by a complex geometry.
- Diffusion channels are much smaller than other scales in system.
- Multiple interacting gas producing and gas absorbing materials.
- Separated time scales: fast reactions, slower diffusion.
- Two diffusive time scales: surface (faster) and bulk (slower)

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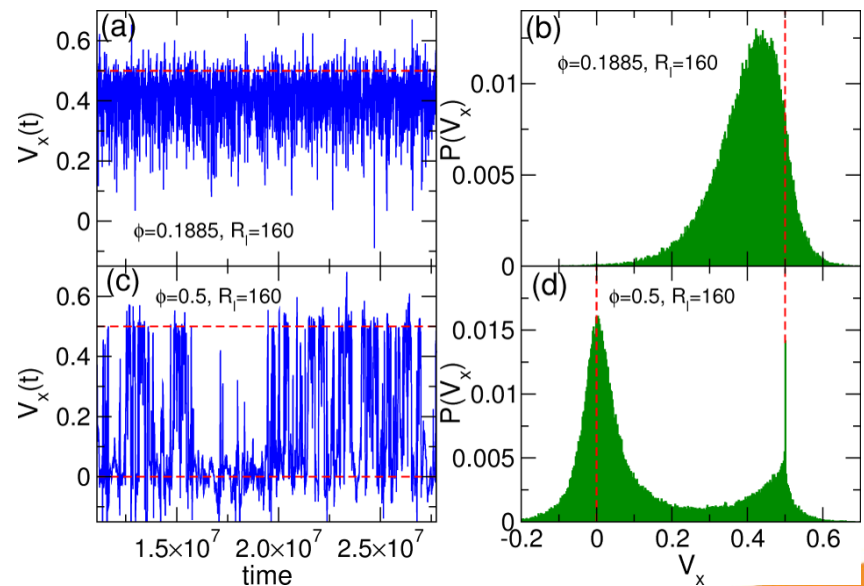
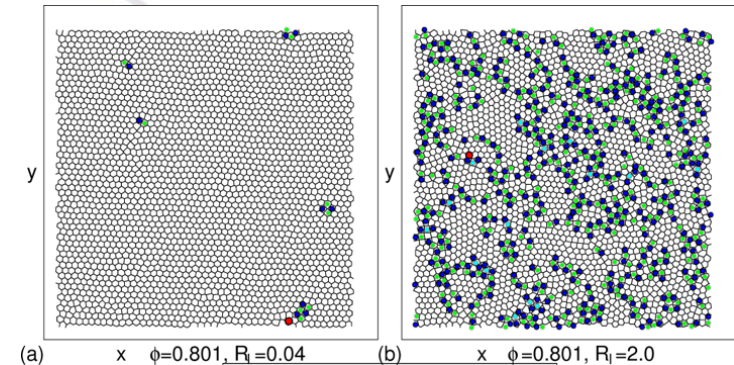
Challenges in Understanding Aging

- System is out of equilibrium so many thermodynamic concepts do not apply.
- Behavior often dominated by rare “worst case” events instead of average events (failure of central limit theorem).
- Existence of a threshold can produce very abrupt behavior change.
- Behavior depends on time history of system (lack of state variables).

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Heterogeneity

- Average bulk response of material not representative of actual response inside material.
- Bulk behavior may be determined by properties of a few local areas that are especially strong or weak.
- Behavior is difficult to model and predict.

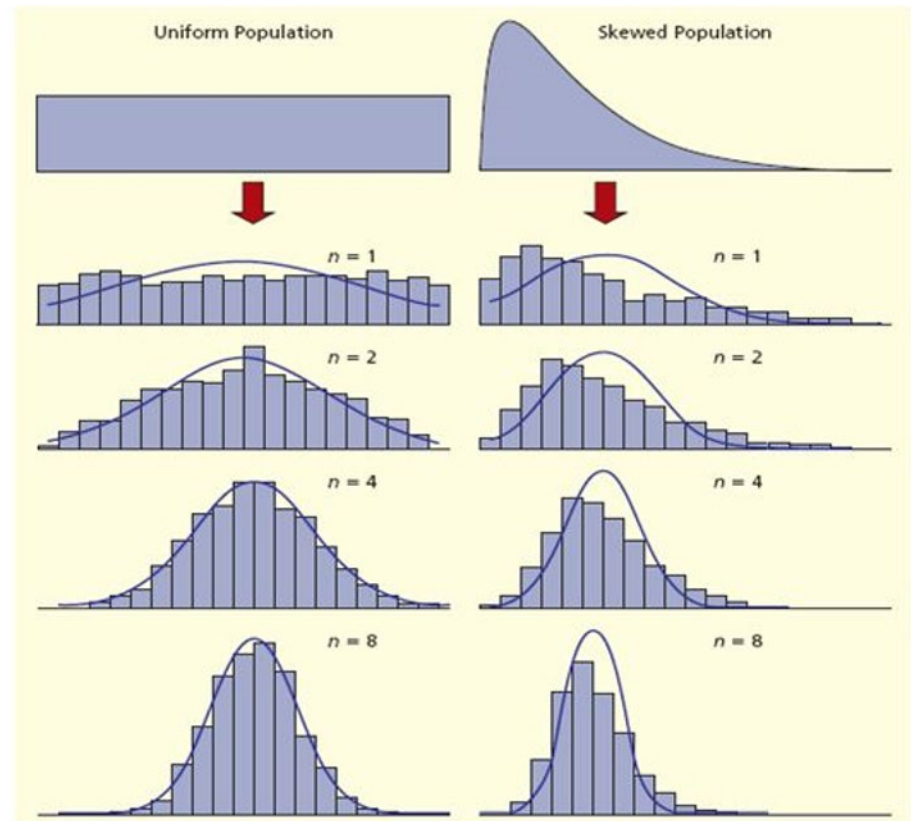


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Phys. Rev. E 91, 032313 (2015)

Failure of the central limit theorem

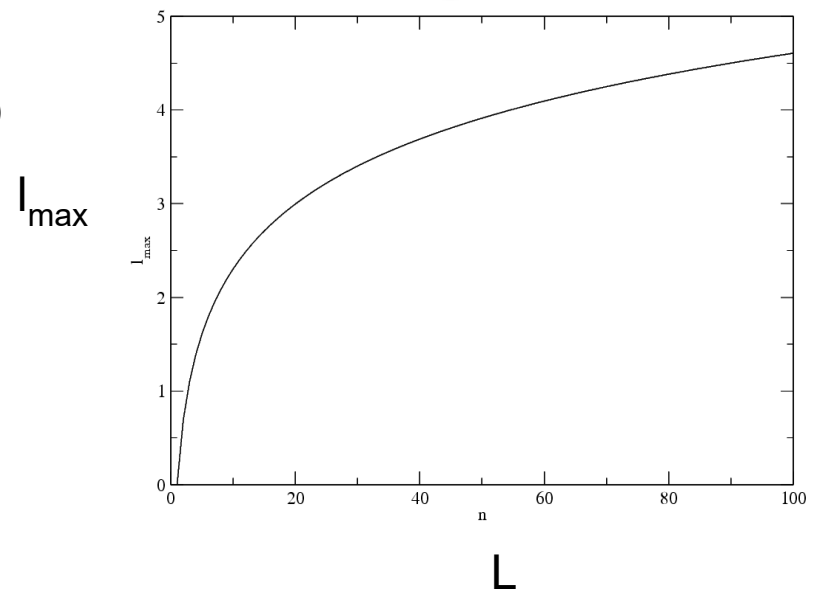
- Typically, as the number of samples increases, behavior tends toward the average.



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Failure of the central limit theorem

- If extreme events dominate behavior (e.g., weakest link), most extreme event becomes more extreme as number of samples increases. (Weibull)

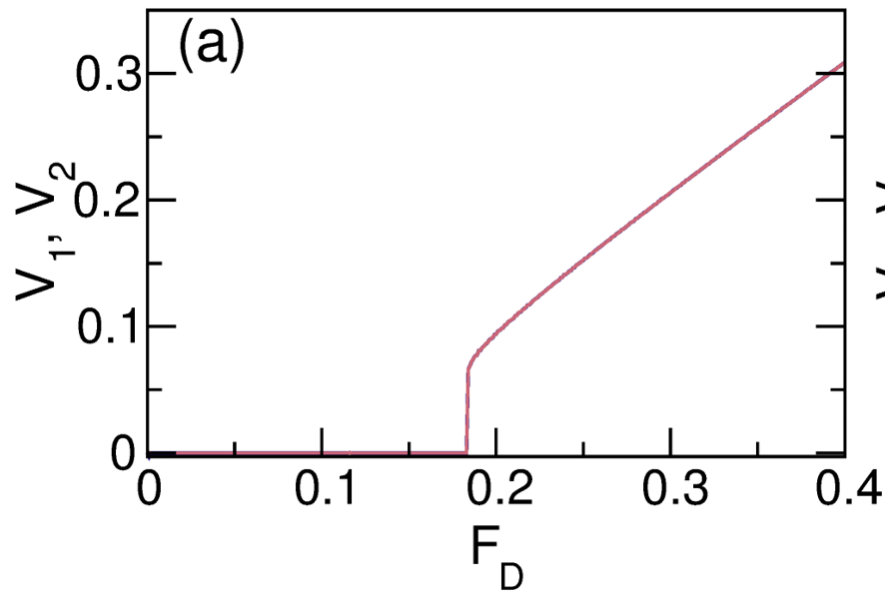


$$l_{\max} = a_0 \ln n.$$

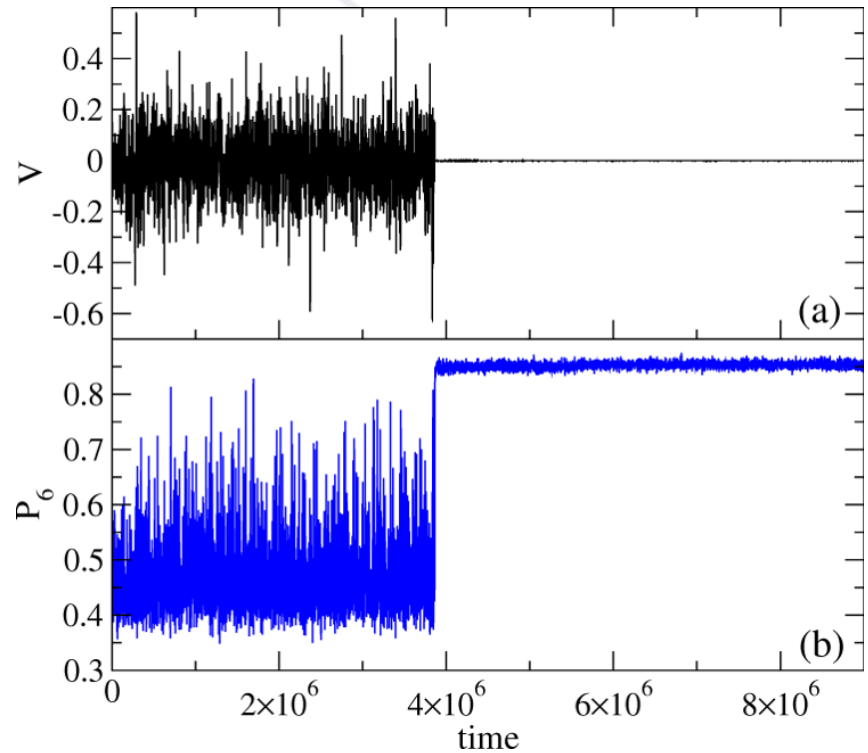
$$G_n(x) = \int_{-\infty}^x g_n(x) dx = 1 - (1 - F(x))^n.$$

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Thresholds and transients



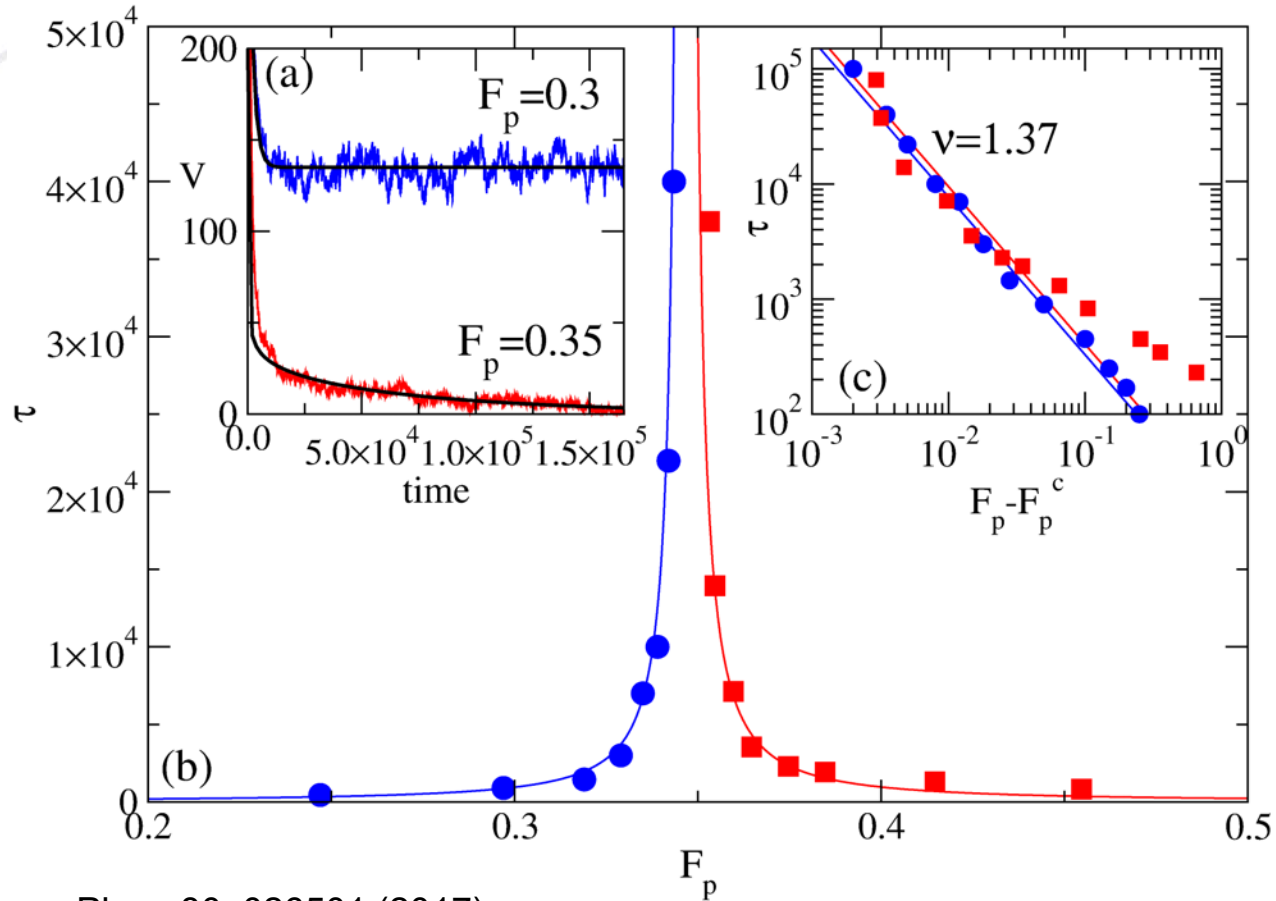
Rep. Prog. Phys. 80, 026501 (2017)



Soft Matter 10, 7502 (2014)

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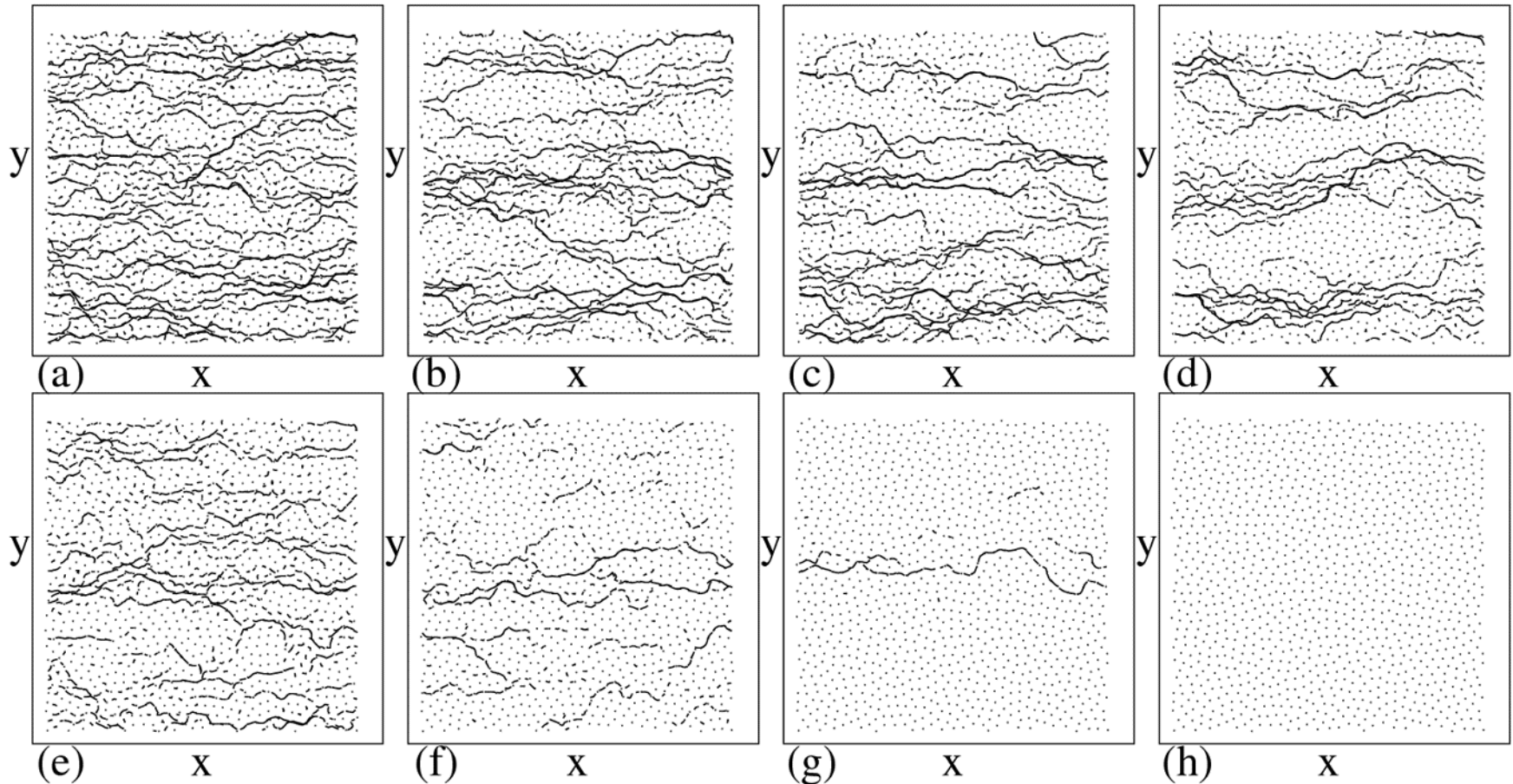
Diverging time scale



Rep. Prog. Phys. 80, 026501 (2017)

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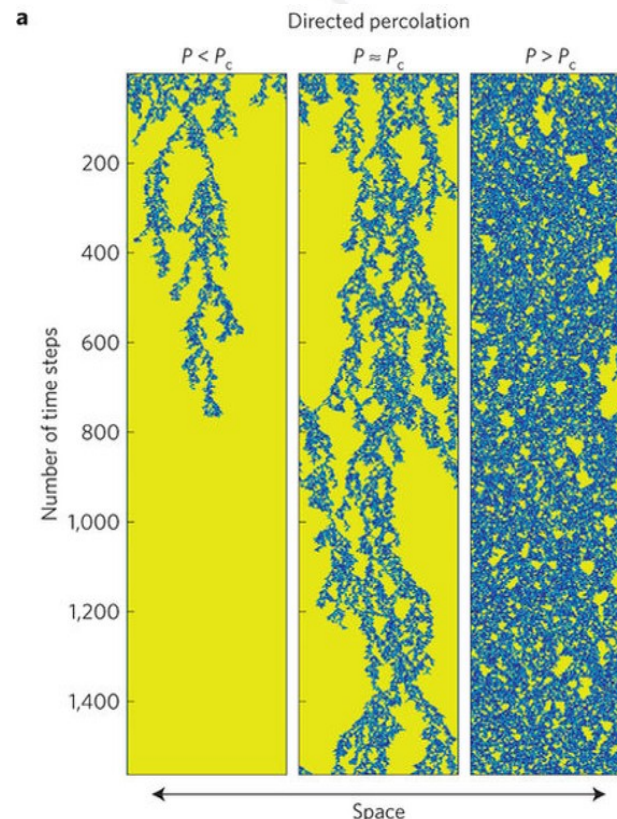
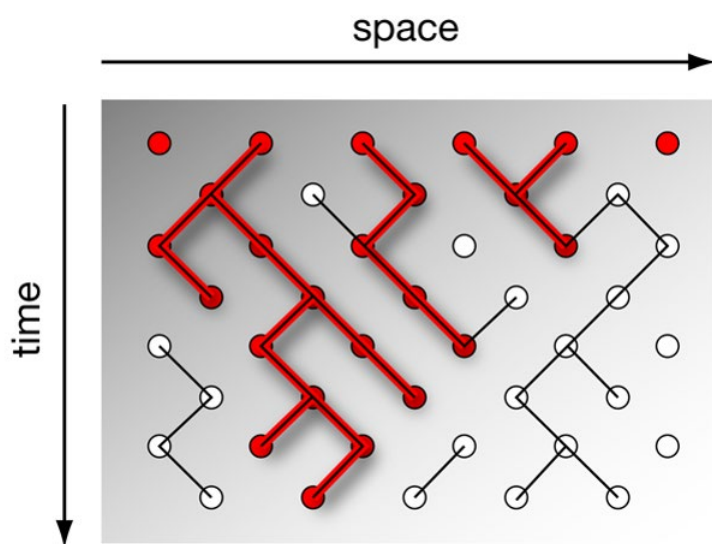
Absorbing phase transition



Phys. Rev. Lett. 103, 168301 (2009)

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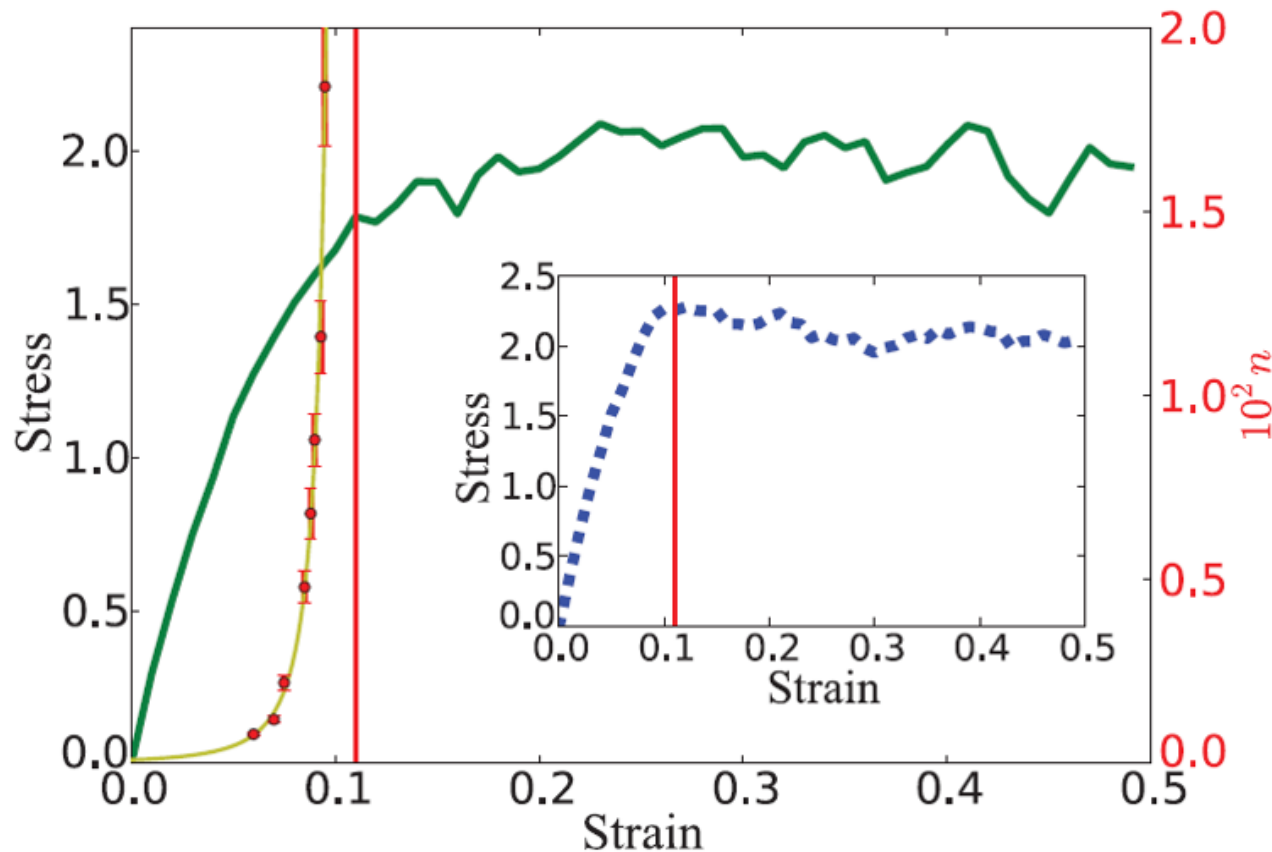
Absorbing phase transition (Directed percolation) from fluctuating to nonfluctuating state



M. Kohl et al, Nat. Commun. 7, 11817 (2016).

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Absorbing phase transition in metallic glass



Rep. Prog. Phys. 80, 026501 (2017)

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Summary

- DRACO designed for multi-physics reaction-diffusion when narrow channels strongly constrain gas motion.
- Tools from nonequilibrium statistical mechanics can be applied to aging problems.
- Extreme value statistics: when behavior dominated by rare events.
- Threshold processes: when sudden changes of behavior occur.
- Absorbing phase transitions: associated with diverging time scales, long transients, and strong history dependence.

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